TITLE: COMPUTATIONAL AND EXPERIMENTAL MODELING OF SLURRY-BUBBLE COLUMN REACTORS

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ABSTRACT

OBJECTIVE

This project is a collaborative effort between two universities (Akron University and Illinois Institute of Technology) and two industries (UOP and Energy International). The overall objective of this research is to develop predictive hydrodynamic models for gas-liquid-solid catalyst reactors using computational fluid dynamics (CFD) techniques. The work plan involves a combination of computational, experimental and theoretical studies with a feedback mechanism to correct model deficiencies. The tasks involve : 1- Development of a CFD code for slurry bubble column reactors. 2- Optimization. 3- Comparison to reactor data. 4- Development of a three dimensional transient CFD code. 5- Measurement of particle turbulent properties. 6- a) Measurement of thermal conductivity of particles in the IIT two story riser. b) Measurements of evaporation rates of liquid nitrogen in the IIT riser.

ACCOMPLISHMENTS TO DATE

Our paper describing the basic approach using kinetic theory to predict the turbulence of catalyst particles in a slurry bubble column reactor, has been published in a refereed journal (Wu and Gidaspow, 2000). The computed slurry height, gas hold up and rate of methanol production agreed with the Department of Energy La Porte pilot plant reactor data. The computed turbulent kinetic energy agreed with IIT measurements using a methanol catalyst and with similar measurements at Ohio State University in a bubble column extrapolated to no particles.

We have invented an alternate technique for computing turbulence in a slurry bubble column. It involves direct numerical simulation of the equations of motion with the measured particular viscosity as an

input. We have computed the flow profiles, particle concentration profiles and Reynolds stresses for an IIT slurry bubble column. We see good agreement between the computations and the measurements done earlier at IIT. The computations were done using our previous two dimensional three phase code and a newly developed three dimensional version. This work will be reported in the Ph.D. thesis by Diana Matonis, to be defended Apr. 27, 2000.
Measurements of thermal conductivity of catalyst particles in the IIT riser were completed. The IIT riser was redesigned to eliminate asymmetries, similarly to the Sandia National Laboratory riser, sponsored by the Multiphase Fluid Dynamics Research Consortium. Our CCD camera system was used to measure Reynolds stresses for 450 μm glass beads.

SIGNICANCE TO FOSSIL ENERGY PROGRAMS

There is a need to find domestic alternative sources for the fast depleting conventional petroleum and gas for economics and national security reasons. Coal liquefaction, direct and indirect, appears to be a good candidate.
Indirect liquefaction is a two stage process that employs a gasification technology to first produce synthesis gases from coal. The synthesis gases are then converted to various hydrocarbon products and oxygenates in a slurry bubble column reactor in the presence of catalyst and solvent. The indirect liquefaction technology is being developed by DOE/Air Products at the La Porte Alternative Fuels Development Unit, Exxon, Shell, Sasol and Energy International Corporation, a subsidiary of Williams Field Services.

PLANS FOR COMING YEAR

- Completions of turbulence studies in the IIT riser.
- Injection of liquid nitrogen into the IIT riser and measurement of catalyst concentration distribution with flow of liquid nitrogen.
- Addition of the Fischer-Tropsch kinetics into the CFD codes.
- Preparation of a major paper on the computation of turbulence in slurry bubble column reactors.
- Suggestions for design improvements.

ARTICLES AND PRESENTATIONS

Journal Articles

- Wu Y. and D. Gidaspow, "Hydrodynamic simulation of methanol synthesis in gas-liquid slurry bubble column reactors", Chem. Eng. Sci., 55, 573-587, 2000.

Conference Presentations

- Gidaspow D., "Fluidized Bed Hydrodynamics and Direct Contact Heat Transfer using Kinetic Theory", Festschrift session, 33rd National Heat Transfer Conference, Albuquerque, New Mexico, Aug. 15-17, 1999.
- Gidaspow D., Wu Y. and R. Mostofi, "Turbulence of Particles in a CFB and Slurry Bubble Columns using Kinetic Theory", Fluidization and Fluid-Particle Systems Preprint Volume, AIChE, pp. 261-266, AIChE Annual meeting, Dallas, Texas, Oct. 31-Nov. 5, 1999.
- Gidaspow D., Mostofi R., Tartan M., Vijayaraghavan K., Sharma B., Matonis D. and Y.S. Shin, "Computation and Measurement of Structure and Turbulence in Risers and Bubbling Beds", Multiphase Fluid Dynamics Research Consortium Annual Meeting, Albuquerque, New Mexico, Apr. 12, 2000.